3-Methylhexane

589-34-4 | DTXSID3044334

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 305 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.50e-01

Confidence level: 6.99e-01

Nearest Neighbors from the Training Set

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Ethylbenzene
Measured: 170
Predicted: 271

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Propylbenzene
Measured: 741
Predicted: 859

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Styrene
Measured: 912
Predicted: 358

Image not found

para-Xylene
Measured: 257
Predicted: 246

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4-Methylaniline
Measured: 79.4
Predicted: 104